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# Grain Boundaries in Diamond: From First Principles to Macroscopic Descriptions

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Atomic-scale structures and energies of <001> and <011> symmetrical tilt grain boundaries (GBs) in diamond have been calculated by combining atomistic modeling techniques using an analytic potential, first-principles calculations and a mesoscopic continuum mechanics approach. The mesoscopic disclination-structural units model uses as input interface structures and energies of a few reference GBs for the prediction of energies and stress fields over an entire range of misorientation. An empirical bond-order potential is used to obtain GB structures, verify the validity of the disclination-structural units model for covalent crystals and determine the spatial extent of stress fields. The latter defines the cell size for the first principles calculations. The energies of reference GBs are obtained from first-principles pseudopotential density functional calculations. Modifications of the disclination-structural units model that take into account structural peculiarities of interfaces in covalent crystals will be discussed.

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